Energy approach to Coulomb and log gases

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The classical Coulomb gas Hamiltonian

\[ H_n(x_1, \ldots, x_n) = \sum_{i \neq j} w(x_i - x_j) + n \sum_{i=1}^{n} V(x_i) \quad x_i \in \mathbb{R}^d \]

\[ w(x) = \begin{cases} 
\frac{1}{|x|^{d-2}} & \text{if } d \geq 3 \\
- \log |x| & \text{if } d = 1, 2
\end{cases} \]

\[ -\Delta w = c_d \delta_0 \quad \text{if } d \geq 2 \]

\( V \) confining potential, sufficiently smooth and growing at infinity

With temperature: Gibbs measure

\[ d\mathbb{P}_{n,\beta}(x_1, \ldots, x_n) = \frac{1}{Z_{n,\beta}} e^{-\frac{\beta}{2} H_n(x_1, \ldots, x_n)} dx_1 \ldots dx_n \quad x_i \in \mathbb{R}^d \]

\( Z_{n,\beta} \) partition function

Limit \( n \to \infty \)?
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\[ w(x) = \frac{1}{|x|^{d-2}} \text{ if } d \geq 3 = -\log|x| \text{ if } d = 1, 2 \]

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Limit \( n \to \infty \)?
Motivations

- statistical mechanics
- connection to random matrices (first noticed by Wigner, Dyson)
  \( d = 1 \) Coulomb kernel: completely solvable Lenard, Aizenman-Martin, Brascamp-Lieb
  \( d = 1 \) log gas or \( d \geq 2 \) Coulomb gas Lieb-Narnhofer '75, Penrose-Smith '72, Sari-Merlini '76, Alastuey-Jancovici '81, Frohlich-Spencer '81, Jancovici-Lebowitz-Manificat '93, Kiessling '93, Kiessling-Spohn '99, Chafai-Gozlan-Zitt '13, Valko-Virag '09, Bourgade-Erdős-Yau '12, Scherbina '14, Beckerman-Figalli-Guionnet '14...
- weighted Fekete points, Fekete points on spheres
  Rakhmanov-Saff-Zhou

\[
\min_{x_1, \ldots, x_n \in S^d} \left( - \sum_{i \neq j} \log |x_i - x_j| \right)
\]

- Riesz \( s \)-energy

\[
\min_{x_1 \ldots x_n \in S^d} \sum_{i \neq j} \frac{1}{|x_i - x_j|^s}
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cf. Smale’s 7th problem originating in computational complexity
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The mean field limit

- For \((x_1, \ldots, x_n)\) minimizing \(H_n\), one can prove
  \[
  \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i} = \mu_0 \quad \lim_{n \to \infty} \frac{\min H_n}{n^2} = \mathcal{E}(\mu_0)
  \]

  where \(\mu_0\) is the unique minimizer of
  \[
  \mathcal{E}(\mu) = \int_{\mathbb{R}^d \times \mathbb{R}^d} w(x - y) \, d\mu(x) \, d\mu(y) + \int_{\mathbb{R}^d} V(x) \, d\mu(x).
  \]

  among probability measures.

  \(\mathcal{E}\) has a unique minimizer \(\mu_0\) among probability measures, called the *equilibrium measure* (Frostman 50's potential theory)

- Denote \(\Sigma = \text{Supp}(\mu_0)\). We assume \(\Sigma\) is compact with \(C^1\) boundary and if \(d \geq 2\) that \(\mu_0\) has a density bounded above and below on \(\Sigma\) with is \(C^1\) in \(\Sigma\).

- With temperature, a corresponding LDP can be proven (Petz-Hiai, Ben Arous-Zeitouni, Ben Arous-Guionnet, Chafai-Gozlan-Zitt)

- We look at next order terms by expanding \(\sum_{i=1}^{n} \delta_{x_i}\) as \(n \mu_0 + (\sum_{i=1}^{n} \delta_{x_i} - n \mu_0)\) and inserting into \(H_n\).
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\lim_{n \to \infty} \frac{\sum_{i=1}^{n} \delta_{x_i}}{n} = \mu_0 \quad \text{and} \quad \lim_{n \to \infty} \frac{\min H_n}{n^2} = \mathcal{E}(\mu_0)
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  \lim_{n \to \infty} \frac{\sum_{i=1}^{n} \delta_{x_i}}{n} = \mu_0 \quad \lim_{n \to \infty} \frac{\min H_n}{n^2} = E(\mu_0)
  \]

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Approach

- In Sandier-S, we developed an essentially 2D approach to the problem, inspired from our work on vortices in Ginzburg-Landau. Relies on “ball construction methods" introduced by Jerrard, Sandier in the context of GL. Works for $-\log$ in $d = 1, 2$.

- In Rougerie-S we developed an approach valid for any $d \geq 2$, based instead on Onsager’s lemma (smearing out the charges). (Previous related work Rougerie-S-Yngvason)
Next order expansion of $\min H_n$ and $Z_{n, \beta}$

**Theorem (ground state energy, Rougerie-S $d \geq 2$, Sandier-S $d = 1, 2$)**

*Under suitable assumptions on $V$, as $n \to \infty$ we have*

$$
\min H_n = \begin{cases}
  n^2 E(\mu_0) + n^{2-2/d} \left( \frac{\alpha_d}{c_d} \int \mu_0^{2-2/d}(x) dx + o(1) \right) & \text{if } d \geq 3 \\
  n^2 E(\mu_0) - \frac{n}{2} \log n + n \left( \frac{\alpha_2}{2\pi} - \frac{1}{2} \int \mu_0(x) \log \mu_0(x) dx + o(1) \right) & \text{if } d = 2 \\
  n^2 E(\mu_0) - n \log n + n \left( \frac{\alpha_1}{2\pi} - \int \mu_0(x) \log \mu_0(x) dx + o(1) \right) & \text{if } d = 1
\end{cases}
$$

*where $\alpha_d = \min \mathcal{W}$ depends only on $d$ (see later).*
Theorem (ctd, free energy expansion)

Assume there exists $\beta_1 > 0$ such that

\[
\begin{aligned}
\int e^{-\beta_1 V(x)/2} \, dx &< \infty \text{ when } d \geq 3 \\
\int e^{-\beta_1 \left( \frac{V(x)}{2} - \log |x| \right)} \, dx &< \infty \text{ when } d = 1, 2.
\end{aligned}
\]

If $d \geq 3$ and $\beta \geq cn^{2/d-1}$ or $d = 1, 2$ and $\beta \geq c(\log n)^{-1}$

\[
\left| -\frac{2}{\beta} \log Z_{n,\beta} - \min H_n \right| \leq o(n^{2-2/d}) + C \frac{n}{\beta}.
\]

$\Rightarrow$ transition regime $\beta \gg n^{2/d-1}$ if $d \geq 3$, $\beta \gg 1$ if $d = 1, 2$
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$\Rightarrow$ transition regime $\beta \gg n^{2/d - 1}$ if $d \geq 3$, $\beta \gg 1$ if $d = 1, 2$
After blow up the points should interact according to a Coulomb interaction, but screened by a fixed background charge: jellium
Some notation

- Start with the potential generated by $\sum_{i=1}^{n} \delta_{x_i} - n\mu_0$, and blow up.
- Set $\mu'_0(x') = \mu_0(x') n^{-1/d}$, blown-up background density and for $x_1, \ldots, x_n$, set $x'_i = n^{1/d} x_i$ and

$$h_n(x') = -c_d \Delta^{-1} \left( \sum_{i=1}^{n} \delta_{x_i'} - \mu'_0 \right) = w * \left( \sum_{i=1}^{n} \delta_{x_i'} - \mu'_0 \right)$$

- For any $x, \eta > 0$, let $\delta_{x}^{(\eta)} = \frac{1}{|B(0,\eta)|} \mathbb{1}_{B(x,\eta)}$, "smeared out" Dirac mass at scale $\eta$
- **Newton's theorem**: the potentials generated by $\delta_0$ and $\delta_0^{(\eta)}$ (i.e. $w * \delta_0 = w$ and $w * \delta_0^{(\eta)}$) coincide outside $B(0, \eta)$, and $w \geq w * \delta_0^{(\eta)}$. Then

$$h_{n,\eta}(x') = -c_d \Delta^{-1} \left( \sum_{i=1}^{n} \delta_{x_i'}^{(\eta)} - \mu'_0 \right) = w * \left( \cdots \right)$$

can be defined unambiguously and coincides with $h_n$ outside $\cup_i B(x'_i, \eta)$. 
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Splitting formula

As in Onsager's lemma (used in “stability of matter", cf Lieb-Oxford, Lieb-Seiringer): from Newton’s theorem we have

\[ \sum_{i \neq j} w(x_i - x_j) \geq \sum_{i \neq j} \int \int w(x - y) \delta^{(\ell)}_{x_i}(x) \delta^{(\ell)}_{x_j}(y) \]

\[ = \int \int w(x - y) \left( \sum_{i=1}^{n} \delta^{(\ell)}_{x_i}(x) \right) \left( \sum_{j=1}^{n} \delta^{(\ell)}_{x_j}(y) \right) - n \int \int w(x - y) \delta^{(\ell)}_{0}(x) \delta^{(\ell)}_{0}(y) \]

\[ \text{total interaction between smeared-out charges} \]

\[ \text{cst self-interaction term} = \kappa_d c_d^{-1} w(\ell) \]

Insert splitting \( \sum_{i=1}^{n} \delta^{(\ell)}_{x_i} = n \mu_0 + \left( \sum_{i=1}^{n} \delta^{(\ell)}_{x_i} - n \mu_0 \right) \) and characterization of equilibrium measure \( \mu_0 \):

\[ w \ast \mu_0 + \frac{1}{2} V = \zeta + \left( \frac{1}{2} \mathcal{E}(\mu_0) + \int \int w(x - y) d\mu_0(x) d\mu_0(y) \right) \]

for some function \( \zeta \geq 0, \zeta = 0 \) in \( \Sigma \).

Then choose \( \ell = \eta n^{-1/d} \) and blow-up everything by \( n^{1/d} \).
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Then choose \( \ell = \eta n^{-1/d} \) and blow-up everything by \( n^{1/d} \).
Proposition (Splitting formula)

For $d \geq 2$, for any $n$, $(x_1, \ldots, x_n)$, $\eta > 0$,

$$H_n(x_1, \ldots, x_n) \geq n^2 \mathcal{E}(\mu_0) - \left(\frac{n}{2} \log n\right) 1_{d=2}$$

$$+ n^{1-2/d} \left[ \frac{1}{C_d} \left( \int_{\mathbb{R}^d} |\nabla h_n,\eta|^2 - n\kappa_d w(\eta) \right) - C\eta^2 \right] + 2n \sum_{i=1}^{n} \zeta(x_i).$$

The next step is to study the term in brackets and take its limit $n \to \infty$, then $\eta \to 0$.

Dimension 1 is treated in the same way after imbedding the real line into the plane and considering

$$h_n(x', y') = w * \left( \sum_{i} \delta_{(x'_i,0)} - \mu'_0(x')\delta_{y'=0} \right) \quad w = -\log |\cdot|$$

equivalent to taking Stieltjes transform
Proposition (Splitting formula)

For \( d \geq 2 \), for any \( n, (x_1, \ldots, x_n), \eta > 0 \),

\[
H_n(x_1, \ldots, x_n) \geq n^2 \mathcal{E}(\mu_0) - \left( \frac{n}{2} \log n \right) 1_{d=2} \\
+ n^{1-2/d} \left[ \frac{1}{c_d} \left( \int_{\mathbb{R}^d} \left| \nabla h_n, \eta \right|^2 - n \kappa_d w(\eta) \right) - C \eta^2 \right] + 2n \sum_{i=1}^{n} \zeta(x_i) \geq 0.
\]

The next step is to study the term in brackets and take its limit \( n \to \infty \), then \( \eta \to 0 \).

Dimension 1 is treated in the same way after imbedding the real line into the plane and considering

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\]

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The renormalized energy

Recall

\[-\Delta h_n = c_d \left( \sum_{i=1}^{n} \delta_{x_i'} - \mu'_0 \right).\]

Centering the blow-up around a point \( x_0 \in \Sigma \), in the limit \( n \to \infty \) we get solutions to

\[-\Delta h = c_d \left( \sum_{p \in \Lambda} N_p \delta_p - \mu_0(x_0) \right) \leftrightarrow -\Delta h_\eta = c_d \left( \sum_{p \in \Lambda} N_p \delta_p(\eta) - \mu_0(x_0) \right)\]

\( \Lambda \) infinite discrete set of points in \( \mathbb{R}^d \), \( N_p \in \mathbb{N}^* \).
Definition
Let $m > 0$. Call $\overline{A}_m$ the class of $\nabla h$ such that

$$-\Delta h = c_d \left( \sum_{p \in \Lambda} N_p \delta_p - m \right)$$

with $N_p \in \mathbb{N}^*$. 

Definition (Rougerie-S)
Set $K_R = [-R, R]^d$. For $\nabla h \in \overline{A}_m$ we let

$$\mathcal{W}(\nabla h) = \liminf_{\eta \to 0} \left( \limsup_{R \to \infty} \int_{K_R} |\nabla h_\eta|^2 - \kappa_d m w(\eta) \right).$$

Alternate definition by Sandier-S in $d = 1, 2$, originating in Ginzburg-Landau theory.
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Alternate definition by Sandier-S in $d = 1, 2$, originating in Ginzburg-Landau theory.
- If $\mathcal{W}(\nabla h) < +\infty$ then $\lim_{R \to \infty} f_{K_R}(\sum_p N_p \delta_p) = m$

- By scaling, one can reduce to $\overline{A}_1$, with

$$\inf_{\overline{A}_m} \mathcal{W} = m^{2-2/d} \inf_{\overline{A}_1} \mathcal{W} \quad d \geq 3$$

$$= m \left( \inf_{\overline{A}_1} \mathcal{W} - \pi \log m \right) \quad d = 2$$

- $\mathcal{W}$ is bounded below, and has minimizers over $\overline{A}_1$, even sequences of periodic minimizers (with larger and larger period)
The case of the torus

Assume $\Lambda$ is $\mathbb{T}$-periodic. Then $W$ is $+\infty$ unless all $N_p = 1$, and can be written as a function of $\Lambda " = " \{a_1, \ldots, a_M\}$, $M = |\mathbb{T}|$.

$$W(a_1, \cdots, a_M) = \frac{c_d^2}{|\mathbb{T}|} \sum_{j \neq k} G(a_j - a_k) + \text{cst},$$

where $G = $ Green’s function of the torus ($-\Delta G = \delta_0 - 1/|\mathbb{T}|$).
Partial minimization results

Theorem (Sandier-S.)

In dimension $d = 1$ ($w = -\log$), the minimum of $\mathcal{W}$ over all possible configurations is achieved for the lattice $\mathbb{Z}$ ("clock distribution").

In dimension $d = 2$, the minimum of $\mathcal{W}$ over perfect lattice configurations (Bravais lattices) with fixed volume is achieved uniquely, modulo rotations, by the triangular lattice.

Relies on a number theory result of Cassels, Rankin, Ennola, Diananda, 50’s, on the minimization of $\zeta(s) = \sum_{p \in \Lambda} \frac{1}{|p|^s}$. 

\[ \mathbb{R}^2 \]
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\[
\begin{array}{c}
\mathbb{R}^2 \\
\end{array}
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There is no corresponding result in higher dimension! In dimension 3, does the FCC (face centered cubic) lattice play this role?

**Conjecture**

*In dimension 2, the “Abrikosov” triangular lattice is a global minimizer of $W$.***

- This conjecture was made in the context of vortices in the GL model, which form Abrikosov lattices.
- Bétermin shows that this conjecture is equivalent to a conjecture of Brauchart-Hardin-Saff on the order $n$ term in the expansion of the minimal logarithmic energy on $S^2$.
- By our result, solving the conjecture (or identifying $\min W$) is equivalent to computing the $\lim_{\beta \to \infty}$ of the order $n$ term in $\log Z_{n,\beta}$.
- $W$ is a measure of disorder of a given point configuration.
- It allows to control things such as fluctuations of number of points.
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Theorem (Rota Nodari-S)

Let \((x_1, \ldots, x_n) \subset (\mathbb{R}^2)^n\) minimize \(H_n\), and assume the equilibrium measure \(\mu_0 \in L^\infty\), then

- for all \(i\), \(x_i \in \Sigma\)
- letting \(\nu'_n = \sum_i \delta_{x'_i}\), if \(\ell \geq c > 0\) and \(\text{dist}(K_\ell(a), \partial \Sigma') \geq n^{\beta/2} (\beta < 1)\), we have

\[
\limsup_{n \to \infty} \left| \nu'_n(K_\ell(a)) - \int_{K_\ell(a)} \mu'_0(x) \, dx \right| \leq C \ell.
\]

- equidistribution of energy

\[
\limsup_{n \to \infty, \eta \to 0} \left| \int_{K_\ell(a)} |\nabla h'_{n, \eta}|^2 - \kappa_d \nu'_n(K_\ell(a)) w(\eta) \right|

- \int_{K_\ell(a)} \left( \min \mathcal{W} \right) dx \right| \leq o_\ell(\ell^2).
\]
We prove the same for minimizers of $\mathcal{W}$ themselves

Should work also in $d \geq 3$

Compare to Ameur - Ortega Cerda: only first result, with $o(\ell^2)$ error.
The averaged formulation

- Let \((x_1, \ldots, x_n) \in (\mathbb{R}^d)^n\). We denote \(P_n\) the probability, push-forward of the normalized Lebesgue measure on \(\Sigma\) by

\[
\begin{align*}
  \mathbb{P}^n &\rightarrow (x, \nabla h_n(n^{1/d}x + \cdot)) \\
\end{align*}
\]

where \(h_n\) is the potential generated by \(\sum_{i=1}^n \delta_{x_i'} - \mu_0'\).

- If the next order terms in \(H_n\) are bounded by \(Cn^{2-2/d}\), then \(P_n\) is tight and up to a subsequence converges to some probability \(P\).

- \(P\) belongs to the class \(C\) of probabilities on \((x, \nabla h)\)'s such that
  1. The first marginal of \(P\) is the normalized Lebesgue measure on \(\Sigma\), and \(P\) is translation-invariant
  2. For \(P\)-a.e. \((x, \nabla h)\), we have \(\nabla h \in \overline{A}_{\mu_0(x)}\).

- Define then \(\widetilde{W}(P) = \frac{\mid \Sigma \mid}{cd} \int \mathcal{W}(\nabla h) \, dP(x, \nabla h)\)

\[
\min_C \widetilde{W} = \frac{1}{cd} \int_{\Sigma} \min_{\alpha_{\mu_0(x)}} \mathcal{W} \, dx.
\]
Theorem (Rougerie-S)

Let $d \geq 2$, $(x_1, \ldots, x_n) \in (\mathbb{R}^d)^n$ and $P_n$ be as above. Up to extraction of a subsequence, we have $P_n \to P \in \mathcal{C}$ and

$$\liminf_{n \to \infty} n^{2/d-2} \left( H_n(x_1, \ldots, x_n) - n^2 \mathcal{E}(\mu_0) + \left( \frac{n}{2} \log n \right) \mathbb{1}_{d=2} \right) \geq \tilde{\mathcal{W}}(P).$$

This lower bound is sharp, thus for minimizers of $H_n$

$$\liminf_{n \to \infty} n^{2/d-2} \left( \min H_n - n^2 \mathcal{E}(\mu_0) + \left( \frac{n}{2} \log n \right) \mathbb{1}_{d=2} \right) = \min_{\mathcal{C}} \tilde{\mathcal{W}}$$

and $P$ minimizes $\tilde{\mathcal{W}}$ over $\mathcal{C}$ (i.e. $P$-a.e. $(x, \nabla h)$ we have $\nabla h$ minimizes $\mathcal{W}$ over $\overline{A}_{\mu_0(x)}$).

Informally: for minimizers, after blow-up around "almost every point in $\Sigma"", we get in the limit $n \to \infty$ an infinite configuration of points minimizing $\mathcal{W}$ in the corresponding class.
Theorem (Rougerie-S \( d \geq 3 \), Sandier-S \( d = 1, 2 \))

Let \( \bar{\beta} = \limsup_{n \to +\infty} \beta n^{1-2/d} \), assume \( \bar{\beta} > 0 \). Then, there exists \( C_{\bar{\beta}} \) such that \( \lim_{\bar{\beta} \to \infty} C_{\bar{\beta}} = 0 \), and if \( A_n \subset (\mathbb{R}^d)^n \)

\[
\limsup_{n \to \infty} \frac{\log P_{n, \beta}(A_n)}{n^{2-2/d}} \leq -\frac{\beta}{2} \left( \inf_{P \in A_{\infty}} \tilde{\mathcal{W}} - \xi_d - C_{\bar{\beta}} \right)
\]

where

\[
A_{\infty} = \{ P : \exists (x_1, \ldots, x_n) \in A_n, \ P_n \to P \ \text{up to a subsequence} \} .
\]
Extensions (ongoing)

With T. Leblé, full LDP at speed \( n^{2-2/d} \) with rate function

\[
\frac{\beta}{2} \tilde{\mathcal{W}}(P) + \text{Ent}(P)
\]

where \( \text{Ent} \) is the specific relative entropy with respect to a Poisson process (cf. Rassoul Agha - Seppalainen)

- gives the existence of a thermodynamic limit or order \( n \) term in \( \log Z_{n,\beta} \) expansion
- shows crystallization happens for \( \beta \gg n^{2/d-1} \) but not before
With M. Petrache, case of Riesz kernel interaction potential:

\[ H_n(x_1, \ldots, x_n) = \sum_{i \neq j} \frac{1}{|x_i - x_j|^s} + n \sum_{i=1}^{n} V(x_i) \quad d - 2 < s < d \]

similar “renormalized energy" derived for minimizers
Use extension to one more space dimension to replace \( \Delta^\alpha \) by a local operator (Caffarelli-Silvestre)

E. Sandier, S.S. 1D Log Gases and the Renormalized Energy: Crystallization at Vanishing Temperature, *arXiv*


N. Rougerie, S. S. Higher Dimensional Coulomb Gases and Renormalized Energy Functionals, *arXiv*

Thank you for your attention!